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MICROSCOPIC ORIGIN OF LINEAR MAGNETO-OPTICAL EFFECT IN BCC FE

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We present analysis of microscopic origin of magneto-optical spectra from the electronic structure of bcc Fe. The magneto-optical (MO) permittivity spectra are obtained by the WIEN2k code and compared to the corresponding experimental MO Kerr effect spectra. The ab-initio spectra are given by the Kubo formula, i.e., as a result of summation over all pairs of electronic bands and integration over the Brillouin zone that all sum up to the single MO spectrum. We investigate what features of electronic structure contribute to the outgoing total MO spectrum. We have also developed several novel ways of visualizing MO-related phenomena in the Brillouin zone.

It turns out that strong MO signal comes from several isolated k-points in the Brillouin zone, where the band degeneracy is avoided by the spin-orbit interaction. There are two major types of MO contributions determined by the nature of the avoided degeneracy (given by topology of the approaching bands), that contribute differently to the total MO spectrum. Both types are visualized and their contributions to the total spectrum are demonstrated in the form of local MO spectra.

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